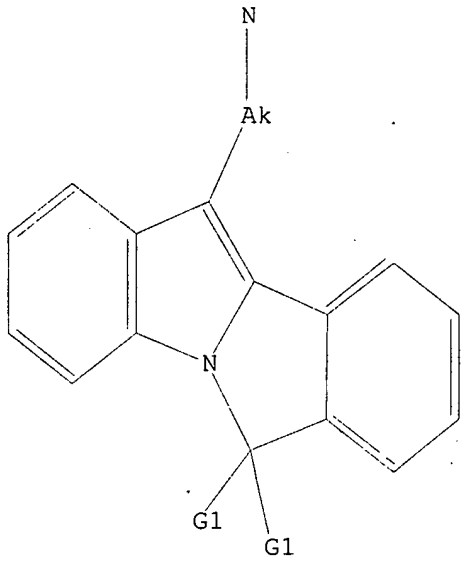
L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1 H,Me,Et,n-Pr,i-Pr

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
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FULL SCREEN SEARCH COMPLETED - 95322 TO ITERATE

100.0% PROCESSED 95322 ITERATIONS 62 ANSWERS
SEARCH TIME: 00.00.02

L2 62 SEA SSS FUL L1

=>
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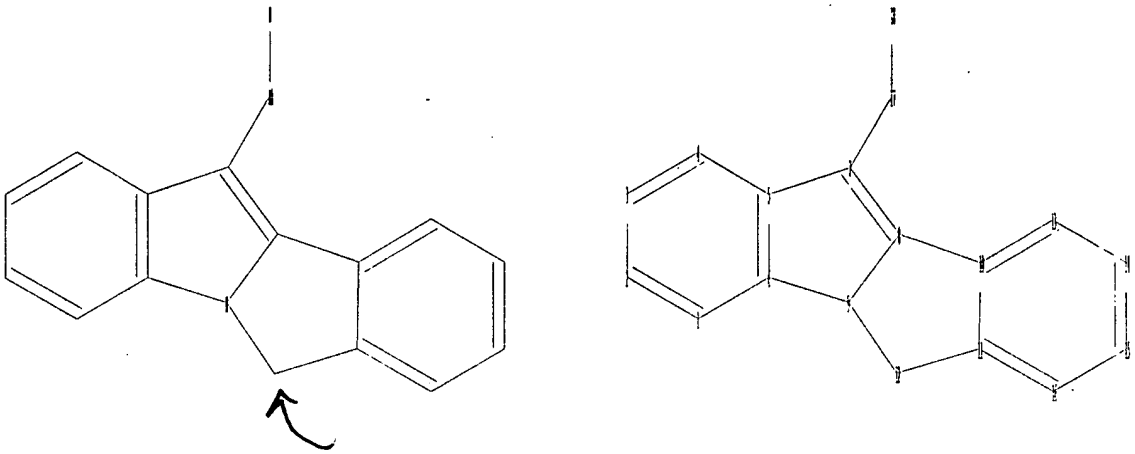


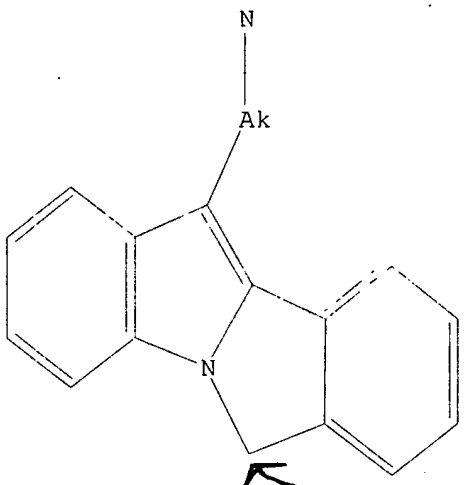
chain nodes :
17
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16
ring/chain nodes :
18
chain bonds :
7-17 17-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 8-10 9-12 10-11 10-13 11-12
11-16 13-14 14-15 15-16
exact/norm bonds :
5-7 6-9 7-8 7-17 8-9 8-10 9-12 11-12 17-18
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-13 11-16 13-14 14-15 15-16
isolated ring systems :
containing 1 :

G1:H,CH3,Et,n-Pr,i-Pr

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS

L3 STRUCTURE UPLOADED

=> d
L3 HAS NO ANSWERS
L3 STR



G1 H,Me,Et,n-Pr,i-Pr

More broad

Structure attributes must be viewed using STN Express query preparation.

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=> s l3 full
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FULL SCREEN SEARCH COMPLETED -    95322 TO ITERATE

100.0% PROCESSED    95322 ITERATIONS                          103 ANSWERS
SEARCH TIME: 00.00.02

L4          103 SEA SSS FUL L3

=> fil caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             333.88     334.09

FILE 'CAPLUS' ENTERED AT 18:30:30 ON 01 NOV 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 1 Nov 2006  VOL 145 ISS 19
FILE LAST UPDATED: 31 Oct 2006  (20061031/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
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They are available for your review at:

http://www.cas.org/infopolicy.html

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=> s l4
L5              11 L4

=> s l2
L6              10 L2

=> d ibib abs hitstr L5 1-11
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Hit # 1 - Instant

2 - 10/518,612

3-11 - all have a  group

@ R_{13}/R_{14} or R_{11}/R_{12} (combined)

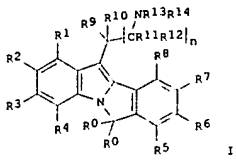
L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:2887 CAPLUS
DOCUMENT NUMBER: 140:77024
TITLE: Preparation of tetracyclic arylalkyl indoles having serotonin receptor affinity
INVENTOR(S): Jasti, Venkateswarlu; Ramakrishna, Venkata Satya Nirogi; Kambhampati, Rama Sastri; Battula, Srinivasa Reddy; Rao, Venkata Satya Veerabhadra Vadlamudi
PATENT ASSIGNEE(S): Suven Pharmaceuticals Ltd., India
SOURCE: PCT Int. Appl., 66 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

Instant App.

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004000845	A1	20031231	WO 2003-IN224	20030619
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2490115	AA	20031231	CA 2003-2490115	20030619
AU 2003249584	A1	20040106	AU 2003-249584	20030619
BR 2003012175	A	20050405	BR 2003-12175	20030619
EP 1537113	A1	20050608	EP 2003-760859	20030619
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1662538	A	20050831	CN 2003-814597	20030619
JP 2006501175	T2	20060112	JP 2004-515426	20030619
US 2005203103	A1	20050915	US 2005-518624	20050513
PRIORITY APPLN. INFO.:			IN 2002-MA476 A	20020621
			WO 2003-IN224 W	20030619

OTHER SOURCE(S): MARPAT 140:77024
GI

L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



I

AB The title compds. [I; R0 = H, alkyl; R1-R12 = H, halo, oxo, thio, etc.; or the adjacent groups like R1 and R2, etc. together with carbon atoms to which they are attached may form 5-7 membered ring which may further contain one or more double bonds and/or one or more heteroatoms such as O, N, S or Se; or R9 and R10 or R11 and R12 together with the carbon atoms to which they are attached may form a 3-6 membered ring which may further contain one or more double bonds and/or one or more heteroatoms such as O, N, S or Se; R13 and R14 = H, alkyl, cycloalkyl, aryl, etc.; or NR13R14 = 3-7 membered heterocyclyl; n = 1-8], useful for treating conditions where a modulation of 5-HT and/or serotonin activity is desired (no data), were prepared Thus, reacting 1-(2'-bromobenzyl)-N,N-dimethyltryptamine with N,N-dimethylacetamide in the presence of PdCl2[P(o-tolyl)3]2 and AcOK afforded 11-(2-N,N-dimethylaminoethyl)-6H-isoindolo[2,1-a]indole. This invention also relates to processes for preparing the compds. I, compns. containing effective amts. of the compound I and the use of such a compound/composition in therapy.

IT 639808-61-0P 639808-62-1P 639808-63-2P
639808-64-3P 639808-65-4P 639808-66-5P
639808-67-6P 639808-68-7P 639808-69-8P
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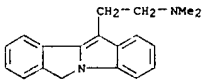
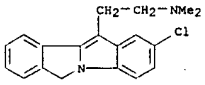
639809-35-1P 639809-38-4P 639809-39-5P
639809-41-9P 639809-42-0P 639809-44-2P
639809-46-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isoindolo[2,1-a]indoles having serotonin receptor affinity)

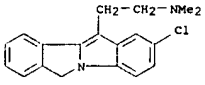
L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 639808-61-0 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 639808-62-1 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-chloro-N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 639808-63-2 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-chloro-N,N-dimethyl-, hydrochloride (9CI) (CA INDEX NAME)



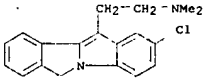
●x HCl

RN 639808-64-3 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-chloro-N,N-dimethyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 639808-62-1
CMF C19 H19 Cl N2

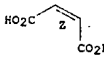
L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



CM 2

CRN 110-16-7
CMF C4 H4 O4

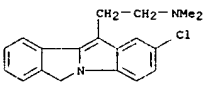
Double bond geometry as shown.



RN 639808-65-4 CAPLUS
CN Butanedioic acid, hydroxy-, compd. with 2-chloro-N,N-dimethyl-6H-isoindolo[2,1-a]indole-11-ethanamine (9CI) (CA INDEX NAME)

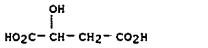
CM 1

CRN 639808-62-1
CMF C19 H19 Cl N2



CM 2

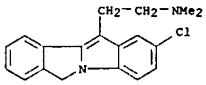
CRN 6915-15-7
CMF C4 H6 O5



RN 639808-66-5 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-chloro-N,N-dimethyl-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CRN 639808-62-1
CMF C19 H19 Cl N2



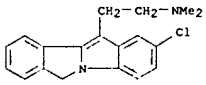
CM 2

CRN 144-62-7
CMF C2 H2 O4

RN 639808-67-6 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-chloro-N,N-dimethyl-, 2-hydroxy-1,2,3-propanetricarboxylate (9CI) (CA INDEX NAME)

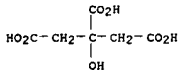
CM 1

CRN 639808-62-1
CMF C19 H19 Cl N2

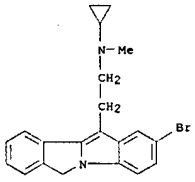


CM 2

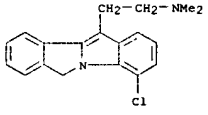
CRN 77-92-9
CMF C6 H8 O7



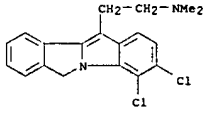
L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 639808-72-3 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-bromo-N-cyclopropyl-N-methyl- (9CI) (CA INDEX NAME)



RN 639808-73-4 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 4-chloro-N,N-dimethyl- (9CI) (CA INDEX NAME)



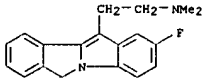
RN 639808-74-5 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 3,4-dichloro-N,N-dimethyl- (9CI) (CA INDEX NAME)



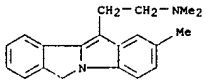
RN 639808-75-6 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 1-chloro-N,N,4-trimethyl- (9CI) (CA INDEX NAME)

L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

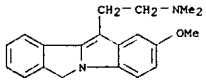
RN 639808-68-7 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-fluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)



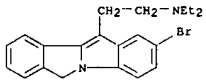
RN 639808-69-8 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, N,N,2-trimethyl- (9CI) (CA INDEX NAME)



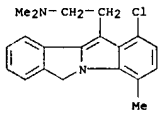
RN 639808-70-1 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-methoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)



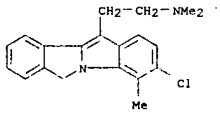
RN 639808-71-2 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-bromo-N,N-diethyl- (9CI) (CA INDEX NAME)



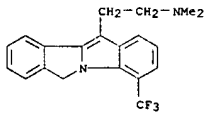
L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



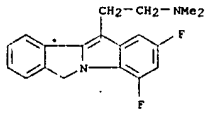
RN 639808-76-7 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 3-chloro-N,N,4-trimethyl- (9CI) (CA INDEX NAME)



RN 639808-77-8 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, N,N-dimethyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

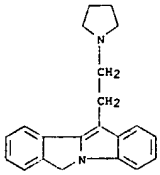


RN 639808-78-9 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2,4-difluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 639808-79-0 CAPLUS
CN 6H-Isoindolo[2,1-a]indole, 11-[2-(1-pyrrolidinyl)ethyl]- (9CI) (CA INDEX

L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
NAME)



RN 639808-80-3 CAPLUS
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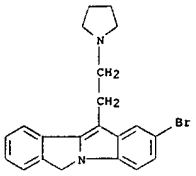

RN 639808-81-4 CAPLUS
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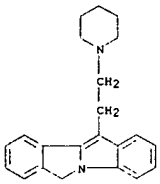
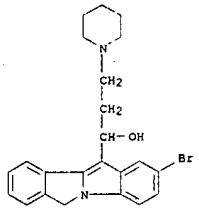
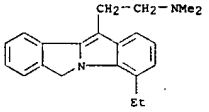


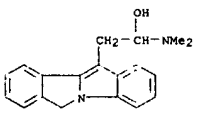
L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 639808-85-8 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 4-ethyl-N,N-dimethyl- (9CI) (CA INDEX NAME)



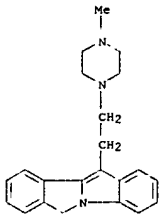
RN 639808-86-9 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanol, α-(dimethylamino)- (9CI) (CA INDEX NAME)



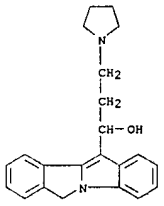
RN 639808-87-0 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 4-methoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)

L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 639808-82-5 CAPLUS
CN 6H-Isoindolo[2,1-a]indole, 11-[2-(4-methyl-1-piperazinyl)ethyl]- (9CI) (CA INDEX NAME)

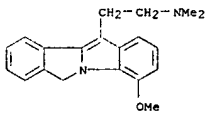


RN 639808-83-6 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-methanol, α-[2-(1-pyrrolidinyl)ethyl]- (9CI) (CA INDEX NAME)

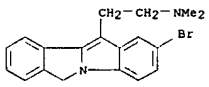


RN 639808-84-7 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-methanol, 2-bromo-α-[2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)

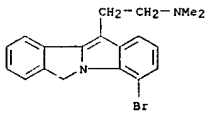
L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



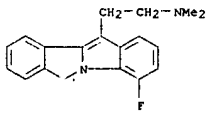
RN 639808-88-1 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-bromo-N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 639808-89-2 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 4-bromo-N,N-dimethyl- (9CI) (CA INDEX NAME)

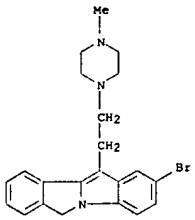


RN 639808-90-5 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 4-fluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 639808-91-6 CAPLUS
CN 6H-Isoindolo[2,1-a]indole, 2-bromo-11-[2-(4-methyl-1-piperazinyl)ethyl]- (9CI) (CA INDEX NAME)

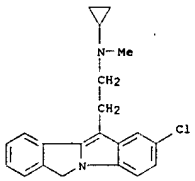
L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 639809-23-7 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-chloro-N-cyclopropyl-N-methyl-, 2-hydroxy-1,2,3-propanetricarboxylate (9CI) (CA INDEX NAME)

CM 1

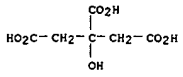
CRN 639809-22-6
CMF C21 H21 Cl N2



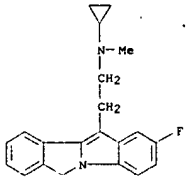
CM 2

CRN 77-92-9
CMF C6 H8 O7

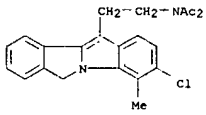
L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 639809-25-9 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, N-cyclopropyl-2-fluoro-N-methyl- (9CI) (CA INDEX NAME)

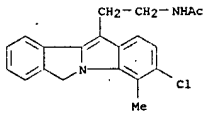


RN 639809-27-1 CAPLUS
CN Acetamide, N-acetyl-N-[2-(3-chloro-4-methyl-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

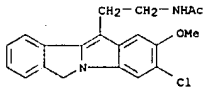


RN 639809-29-3 CAPLUS
CN Acetamide, N-[2-(3-chloro-4-methyl-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

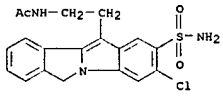
L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



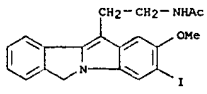
RN 639809-32-8 CAPLUS
CN Acetamide, N-[2-(3-chloro-2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



RN 639809-35-1 CAPLUS
CN Acetamide, N-[2-[2-(aminosulfonyl)-3-chloro-6H-isoindolo[2,1-a]indol-11-yl]ethyl]- (9CI) (CA INDEX NAME)

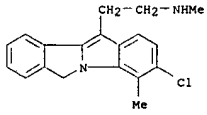


RN 639809-38-4 CAPLUS
CN Acetamide, N-[2-(3-iodo-2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

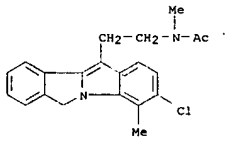


RN 639809-39-5 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 3-chloro-N,4-dimethyl- (9CI) (CA INDEX NAME)

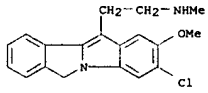
L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



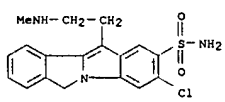
RN 639809-41-9 CAPLUS
CN Acetamide, N-[2-(3-chloro-4-methyl-6H-isoindolo[2,1-a]indol-11-yl)ethyl]-N-methyl- (9CI) (CA INDEX NAME)



RN 639809-42-0 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 3-chloro-2-methoxy-N-methyl- (9CI) (CA INDEX NAME)

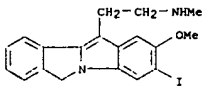


RN 639809-44-2 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-2-sulfonamide, 3-chloro-11-[2-(methylamino)ethyl]- (9CI) (CA INDEX NAME)



RN 639809-46-4 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 3-iodo-2-methoxy-N-methyl- (9CI) (CA INDEX NAME)

L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

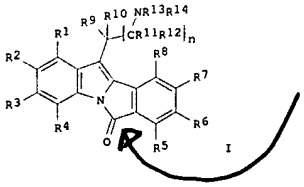
L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:2617 CAPLUS
DOCUMENT NUMBER: 140:77023
TITLE: Preparation of novel tetracyclic arylcarbonyl indoles having serotonin receptor affinity
INVENTOR(S): Jasti, Venkateswarlu; Ramakrishna, Venkata Satya Nirogi, Kambhampati, Rama Sastri; Battula, Srinivasa Reddy; Rao, Venkata Satya Veerabhadra Vadlamudi
PATENT ASSIGNEE(S): Suven Pharmaceuticals Ltd., India; Suven Life Sciences Ltd.
SOURCE: PCT Int. Appl., 63 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004000205	A2	20031231	WO 2003-IN223	20030619
WO 2004000205	A3	20040408		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2490002	AA	20031231	CA 2003-2490002	20030619
AU 2003249583	A1	20040106	AU 2003-249583	20030619
BR 2003012174	A	20050405	BR 2003-12174	20030619
CN 1665815	A	20050907	CN 2003-814592	20030619
JP 2005537239	T2	20051208	JP 2004-515419	20030619
US 2005250834	A1	20051110	US 2005-518612	20050513
PRIORITY APPLN. INFO.:			IN 2002-MA477	A 20020621
			WO 2003-IN223	W 20030619

OTHER SOURCE(S): MARPAT 140:77023
GI

L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



AB The title compds. [I; R1-R12 = H, halo, oxo, thio, etc.; or the adjacent groups like R1 and R2, etc. together with carbon atoms to which they are attached may form 5-7 membered ring which may further contain one or more double bonds and/or one or more heteroatoms such as O, N, S or Se; or R9 and R10 or R11 and R12 together with the carbon atoms to which they are attached may form a 3-6 membered ring which may further contain one or more double bonds and/or one or more heteroatoms such as O, N, S or Se; R13 and R14 = H, alkyl, cycloalkyl, aryl, etc.; or NR13R14 = 3-7 membered heterocyclyl; n = 1-8], useful for treating conditions where a modulation of 5-HT and/or serotonin activity is desired (no data), were prepared

Thus,

reacting 1-(2'-bromobenzoyl)-N,N-dimethyltryptamine with N,N-dimethylacetamide in the presence of PdCl2[P(o-tolyl)3]2 and AcOK afforded 11-(2-N,N-dimethylaminoethyl)-6H-isoindolo[2,1-a]indol-6-one.

This invention also relates to processes for preparing the compds. I, compns.

containing effective amts. of the compound I and the use of such a compound/composition

in therapy.

IT 639805-04-2P 639805-05-3P 639805-06-4P
639805-07-5P 639805-08-6P 639805-09-7P
639805-10-0P 639805-11-1P 639805-12-2P
639805-13-3P 639805-14-4P 639805-15-5P
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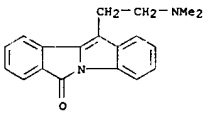
639805-19-9P 639805-20-2P 639805-21-3P
639805-22-4P 639805-24-6P 639805-25-7P
639805-26-8P 639805-27-9P 639805-28-0P
639805-29-1P 639805-30-4P 639805-51-9P
639805-52-0P 639805-53-1P 639805-54-2P
639805-55-3P 639805-56-4P 639805-57-5P
639805-58-6P 639805-59-7P 639805-60-0P
639805-61-1P 639805-62-2P 639805-63-3P
639805-64-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

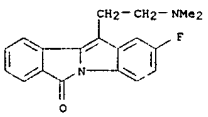
(preparation of isoindolo[2,1-a]indolones having serotonin receptor affinity)

RN 639805-04-2 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)

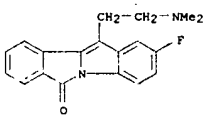
L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 639805-05-3 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-fluoro- (9CI) (CA INDEX NAME)



RN 639805-06-4 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-fluoro-, monohydrochloride (9CI) (CA INDEX NAME)



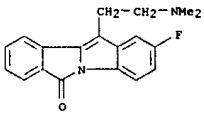
● HCl

RN 639805-07-5 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-fluoro-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 639805-05-3
CMF C19 H17 F N2 O

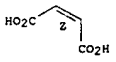
L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



CM 2

CRN 110-16-7
CMF C4 H4 O4

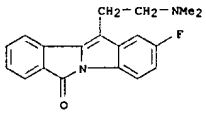
Double bond geometry as shown.



RN 639805-08-6 CAPLUS
CN Butanedioic acid, hydroxy-, compd. with 11-[2-(dimethylamino)ethyl]-2-fluoro-6H-isoindolo[2,1-a]indol-6-one (9CI) (CA INDEX NAME)

CM 1

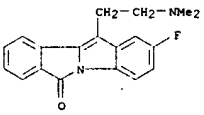
CRN 639805-05-3
CMF C19 H17 F N2 O



CM 2

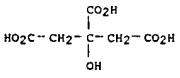
CRN 6915-15-7
CMF C4 H6 O5

L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

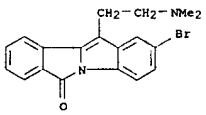


CM 2

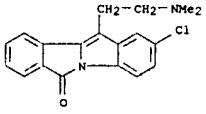
CRN 77-92-9
CMF C6 H8 O7



RN 639805-11-1 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 2-bromo-11-[2-(dimethylamino)ethyl]-(9CI)
(CA INDEX NAME)

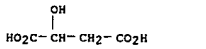


RN 639805-12-2 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 2-chloro-11-[2-(dimethylamino)ethyl]-(9CI) (CA INDEX NAME)



RN 639805-13-3 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 4-chloro-11-[2-(dimethylamino)ethyl]-(9CI) (CA INDEX NAME)

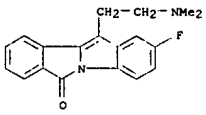
L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 639805-09-7 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-fluoro-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 639805-05-3
CMF C19 H17 F N2 O



CM 2

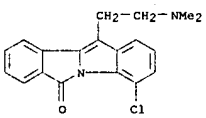
CRN 144-62-7
CMF C2 H2 O4

RN 639805-10-0 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-fluoro-, 2-hydroxy-1,2,3-propanetricarboxylate (9CI) (CA INDEX NAME)

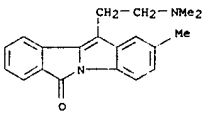
CM 1

CRN 639805-05-3
CMF C19 H17 F N2 O

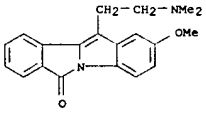
L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



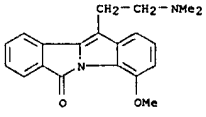
RN 639805-14-4 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-methyl-(9CI) (CA INDEX NAME)



RN 639805-15-5 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-methoxy-(9CI) (CA INDEX NAME)

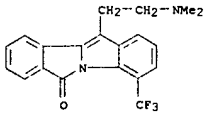


RN 639805-16-6 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-4-methoxy-(9CI) (CA INDEX NAME)

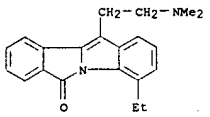


RN 639805-17-7 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-4-

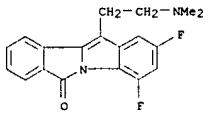
L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 639805-18-8 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-4-ethyl-(9CI)
(CA INDEX NAME)

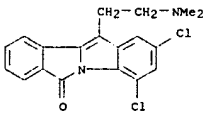


RN 639805-19-9 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2,4-difluoro-(9CI) (CA INDEX NAME)

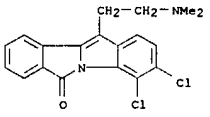


RN 639805-20-2 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 2,4-dichloro-11-[2-(dimethylamino)ethyl]-(9CI) (CA INDEX NAME)

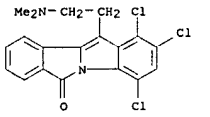
L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



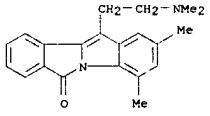
RN 639805-21-3 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 3,4-dichloro-11-[2-(dimethylamino)ethyl]-(9CI) (CA INDEX NAME)



RN 639805-22-4 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 1,2,4-trichloro-11-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)

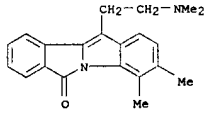


RN 639805-24-6 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2,4-dimethyl-(9CI) (CA INDEX NAME)

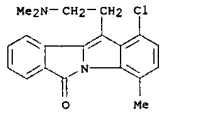


L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

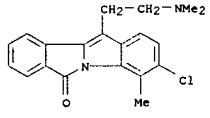
RN 639805-25-7 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-3,4-dimethyl-(9CI) (CA INDEX NAME)



RN 639805-26-8 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 1-chloro-11-[2-(dimethylamino)ethyl]-4-methyl- (9CI) (CA INDEX NAME)

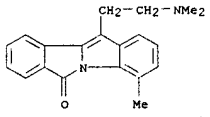


RN 639805-27-9 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 3-chloro-11-[2-(dimethylamino)ethyl]-4-methyl- (9CI) (CA INDEX NAME)

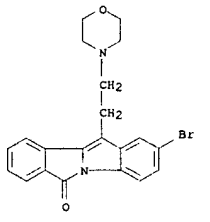


RN 639805-28-0 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-4-methyl-(9CI) (CA INDEX NAME)

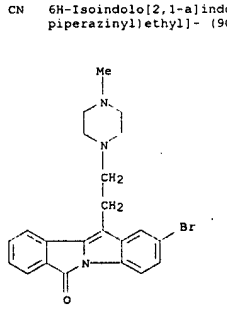
L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 639805-29-1 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 2-bromo-11-[2-(4-morpholinyl)ethyl]-(9CI)
(CA INDEX NAME)

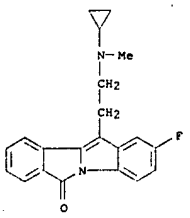


RN 639805-30-4 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 2-bromo-11-[2-(4-methyl-1-piperazinyl)ethyl]- (9CI) (CA INDEX NAME)

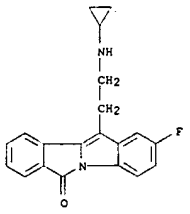


RN 639805-51-9 CAPLUS

L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(cyclopropylmethylamino)ethyl]-2-fluoro- (9CI) (CA INDEX NAME)

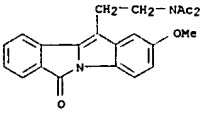


RN 639805-52-0 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(cyclopropylamino)ethyl]-2-fluoro- (9CI) (CA INDEX NAME)

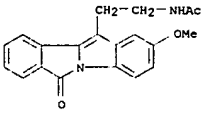


RN 639805-53-1 CAPLUS
CN Acetamide, N-acetyl-N-[2-(2-methoxy-6-oxo-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

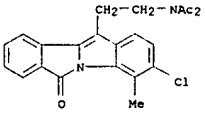
L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 639805-54-2 CAPLUS
CN Acetamide, N-[2-(2-methoxy-6-oxo-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

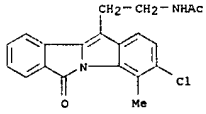


RN 639805-55-3 CAPLUS
CN Acetamide, N-acetyl-N-[2-(3-chloro-4-methyl-6-oxo-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

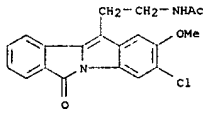


RN 639805-56-4 CAPLUS
CN Acetamide, N-[2-(3-chloro-4-methyl-6-oxo-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

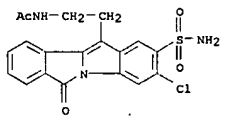
L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



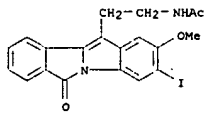
RN 639805-57-5 CAPLUS
CN Acetamide, N-[2-(3-chloro-2-methoxy-6-oxo-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



RN 639805-58-6 CAPLUS
CN Acetamide, N-[2-[2-(aminosulfonyl)-3-chloro-6-oxo-6H-isoindolo[2,1-a]indol-11-yl]ethyl]- (9CI) (CA INDEX NAME)

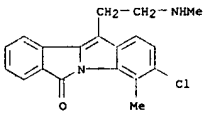


RN 639805-59-7 CAPLUS
CN Acetamide, N-[2-(3-iodo-2-methoxy-6-oxo-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

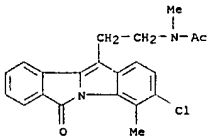


RN 639805-60-0 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 3-chloro-4-methyl-11-[2-

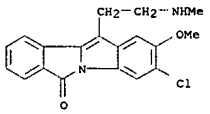
L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
(methylamino)ethyl]- (9CI) (CA INDEX NAME)



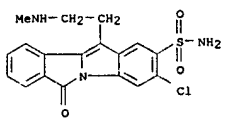
RN 639805-61-1 CAPLUS
CN Acetamide, N-[2-(3-chloro-4-methyl-6-oxo-6H-isoindolo[2,1-a]indol-11-yl)ethyl]-N-methyl- (9CI) (CA INDEX NAME)



RN 639805-62-2 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 3-chloro-2-methoxy-11-[2-(methylamino)ethyl]- (9CI) (CA INDEX NAME)

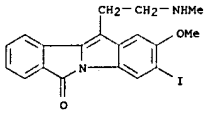


RN 639805-63-3 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-2-sulfonamide, 3-chloro-11-[2-(methylamino)ethyl]-6-oxo- (9CI) (CA INDEX NAME)



L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 639805-64-4 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 3-iodo-2-methoxy-11-[2-(methylamino)ethyl]- (9CI) (CA INDEX NAME)



L5 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

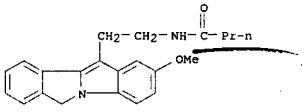
ACCESSION NUMBER: 2003:215250 CAPLUS
DOCUMENT NUMBER: 138:362155
TITLE: Three-Dimensional Quantitative Structure-Activity Relationship Studies on Selected MT1 and MT2 Melatonin Receptor Ligands: Requirements for Subtype Selectivity and Intrinsic Activity Modulation
AUTHOR(S): Rivara, Silvia; Mor, Marco; Silva, Claudia; Zuliani, Valentina; Vacondio, Federica; Spadoni, Gilberto; Bedini, Annalida; Tarzia, Giorgio; Lucini, Valeria; Pannacci, Marilou; Fraschini, Franco; Plazzi, Pier Vincenzo
CORPORATE SOURCE: Dipartimento Farmaceutico, Universita degli Studi di Parma, Parma, I-43100, Italy
SOURCE: Journal of Medicinal Chemistry (2003), 46(8), 1429-1439
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The three-dimensional quant. structure-activity relation comparative mol. field anal. (3D-QSAR CoMFA) approach was applied to some classes of melatonin (MLT) membrane receptor ligands, with the principal aim of exploring the correlation between their steric features and MT2-selective antagonism. Binding data obtained from cloned MT1 and MT2 receptor subtypes were used to develop 3D-QSAR models for agonists and for antagonists at the two receptor subtypes, looking for the structural requirements for receptor subtype selectivity. In particular, we superposed the compds. showing antagonist activity, or very low intrinsic activity at the GTPγS test, following the hypothesis that the occupation of an addnl. pocket positioned out of the plane of MLT is one of the major determinants for MT2 selectivity; the statistical models obtained confirmed this hypothesis. Structure-intrinsic activity relation studies, applied to a set of compds. homogeneously tested, allowed the identification of the structural features whose modulation shifts the behavior from that of the agonist to that of the antagonist. The pocket out of the plane of MLT was identified as one of the key features for obtaining selective MT2 antagonists. The reliability of our statistical models was further confirmed by the correct prediction of the pharmacol. behavior of some N-substituted melatonin derivs., which were prepared and tested on cloned receptor subtypes.

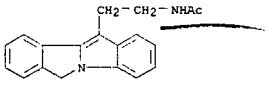
IT 244160-10-9 263865-08-3 263865-09-4
263865-11-8 263865-12-9 263865-13-0
263865-14-1 263865-15-2 263865-16-3
263865-17-4 263865-18-5 263865-19-6
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR of MT1 and MT2 melatonin receptor ligands)

RN 244160-10-9 CAPLUS
CN Butanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

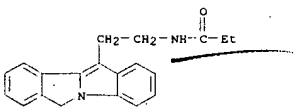
L5 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 263865-08-3 CAPLUS
CN Acetamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

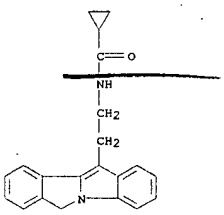


RN 263865-09-4 CAPLUS
CN Propanamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

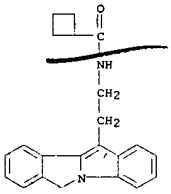


RN 263865-11-8 CAPLUS
CN Cyclopropanecarboxamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

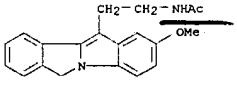
L5 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 263865-12-9 CAPLUS
CN Cyclobutanecarboxamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

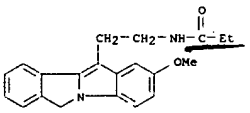


RN 263865-13-0 CAPLUS
CN Acetamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

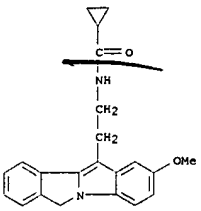


RN 263865-14-1 CAPLUS
CN Propanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

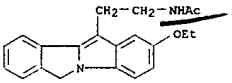
L5 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 263865-15-2 CAPLUS
CN Cyclopropanecarboxamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

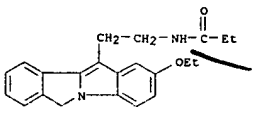


RN 263865-16-3 CAPLUS
CN Acetamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

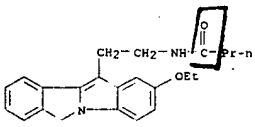


RN 263865-17-4 CAPLUS
CN Propanamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

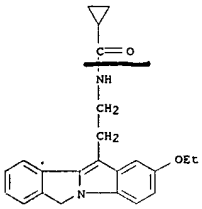
L5 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 263865-18-5 CAPLUS
CN Butanamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



RN 263865-19-6 CAPLUS
CN Cyclopropanecarboxamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

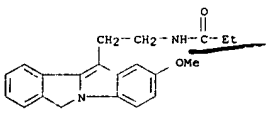
L5 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:10274 CAPLUS
DOCUMENT NUMBER: 136:64149
TITLE: 6H-Isoindolo[2,1-a]indoles or 5,6-dihydroindolo[2,1-a]isoquinolinesas subtype-selective melatonergics for therapeutic use
INVENTOR(S): Jones, Robert M.
PATENT ASSIGNEE(S): Cognetix, Inc., USA
SOURCE: PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

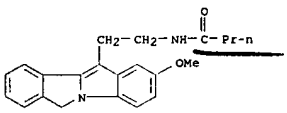
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002000215	A1	20020103	WO 2001-US19958	20010622
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002040018	A1	20020404	US 2001-886609	20010622
PRIORITY APPLN. INFO.:			US 2000-304189P P	20000623
			US 2001-264695P P	20010130

OTHER SOURCE(S): MARPAT 136:64149
AB The invention discloses the use of MT2 selective melatonergics as anticonvulsant agents and as analgesic agents. More specifically, the invention discloses the use of 6H-isoindolo[2,1-a]indoles or 5,6-dihydroindolo[2,1-a]isoquinolines which have melatonin agonist activity and which are selective for the MT2 receptor as anticonvulsant agents or analgesic agents. The invention further relates to the use of 5,6-dihydroindolo[2,1-a]isoquinolines and 6,7-dihydro-5H-benzo[c]azepino[2,1-a]indoles which have melatonin antagonist activity and which are selective for the MT2 receptor as pharmacol. tools for delineation of physiol. responses governed by MT2 receptor activation either by melatonin or selective agonists disclosed herein and for treatment of disorders associated with overprodn. of melatonin such as seasonal affective disorder (SAD) and shift work syndrome. Such melatonin antagonists are also useful for treating Parkinson's Disease.
IT 263865-14-1, CGX 031-120
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(isoindoloindole derivs. and dihydroindoloisoquinoline derivs. as subtype-selective melatonergics for therapeutic use)
RN 263865-14-1 CAPLUS
CN Propanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

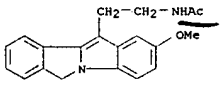
L5 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



IT 244160-10-9, CGX 031139 263865-13-0, CGX 031133
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(phencyclidine-like behavior; isoindoloindole derivs. and dihydroindoloisoquinoline derivs. as subtype-selective melatonergics for therapeutic use)
RN 244160-10-9 CAPLUS
CN Butanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

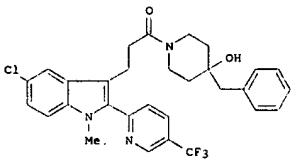


RN 263865-13-0 CAPLUS
CN Acetamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

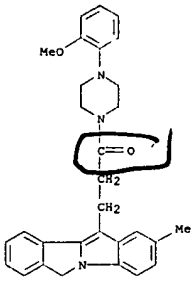
L5 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:321177 CAPLUS
DOCUMENT NUMBER: 135:122368
TITLE: 2-Aryl indole NK1 receptor antagonists: optimization of the 2-Aryl ring and the indole nitrogen substituent
AUTHOR(S): Dinnell, K.; Chicchi, G. G.; Dhar, M. J.; Elliott, J. M.; Hollingworth, G. J.; Kurtz, M. M.; Ridgill, M. P.; Rycroft, W.; Tsao, K.-L.; Williams, A. R.; Swain, C. J.
CORPORATE SOURCE: Department of Medicinal Chemistry, Merck, Sharp and Dohme Research Laboratories, Neuroscience Research Centre, Harlow, Essex, CM20 2QR, UK
SOURCE: Bioorganic & Medicinal Chemistry Letters (2001), 11(9), 1237-1240
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:122368
GI



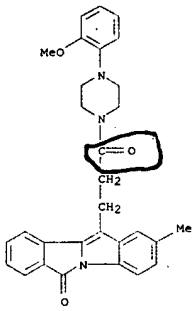
I

AB Novel 2-aryl indole hNK1 receptor ligands were prepared utilizing palladium cross-coupling chemical of a late intermediate as a key step. Compds. with high hNK1 receptor binding affinity and good brain penetration (e.g., I) were synthesized.
IT 351216-15-4P 351216-16-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(optimization of the aryl ring and the indole nitrogen substituent in aryl indole NK1 receptor antagonists)
RN 351216-15-4 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(2-methyl-6H-isoindolo[2,1-a]indol-11-yl)-1-oxopropyl]- (9CI) (CA INDEX NAME)

L5 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



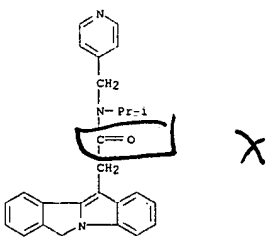
RN 351216-16-5 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(2-methyl-6-oxo-6H-isoindolo[2,1-a]indol-11-yl)-1-oxopropyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

L5 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:246308 CAPLUS
DOCUMENT NUMBER: 135:70637
TITLE: 2-Arylindole-3-acetamides FPP-Competitive inhibitors of farnesyl protein transferase
AUTHOR(S): Trotter, B. W.; Quigley, A. G.; Lumma, W. C.; Sisko, J. T.; Walsh, E. S.; Hamann, C. S.; Robinson, R. G.; Bhimnathwala, H.; Kolodin, D. G.; Zheng, W.; Buser, C. A.; Huber, H. E.; Lobell, R. B.; Kohl, N. E.; Williams, T. M.; Graham, S. L.; Dinsmore, C. J.
CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research Laboratories, West Point, PA, 19486, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2001), 11(7), 865-869
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of 2-arylindole-3-acetamide farnesyl protein transferase inhibitors has been identified. The compds. inhibit the enzyme in a farnesyl pyrophosphate-competitive manner and are selective for farnesyl protein transferase over the related enzyme geranylgeranyltransferase-I. A representative member of this series of inhibitors demonstrates equal effectiveness against HDJ-2 and K-Ras farnesylation in a cell-based assay when geranylgeranylation is suppressed.
IT 347373-82-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(arylindole acetamides farnesyl pyrophosphate-competitive inhibitors of farnesyl protein transferase)
RN 347373-82-4 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-acetamide, N-(1-methylethyl)-N-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR

L5 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

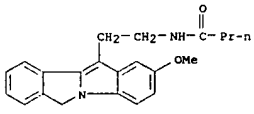
L5 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:185117 CAPLUS
DOCUMENT NUMBER: 132:273842
TITLE: Mapping the Melatonin Receptor. 6. Melatonin Agonists and Antagonists Derived from 6H-Isoindolo[2,1-a]indoles, 5,6-Dihydroindolo[2,1-a]isoquinolines, and 6,7-Dihydro-5H-benzo[c]azepino[2,1-a]indoles
AUTHOR(S): Faust, Ruediger; Garratt, Peter J.; Jones, Rob; Yeh, Li-Kuan; Tsotinis, Andrew; Panoussopoulou, Maria; Calogeropoulou, Theodora; Teh, Muy-Teck; Sugden, David
CORPORATE SOURCE: Department of Chemistry, University College London, London, WC1H 0AJ, UK
SOURCE: Journal of Medicinal Chemistry (2000), 43(6), 1050-1061
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 6H-Isoindolo[2,1-a]indoles, 5,6-dihydroindolo[2,1-a]isoquinolines, and 6,7-dihydro-5H-benzo[c]azepino[2,1-a]indoles have been prepared as melatonin analogs to investigate the nature of the binding site of the melatonin receptor. The affinity of analogs was determined in a radioligand binding assay using cloned human mt1 and MT2 receptor subtypes expressed in NIH 3T3 cells. Agonist and antagonist potency was measured using the pigment aggregation response of a clonal line of Xenopus laevis melanophores. The 2-methoxyisoindolo[2,1-a]indoles showed much higher binding affinities than the parent isoindoles and whereas 2-methoxyisoindolo[2,1-a]indoles were agonists in the functional assay, its cyclopropanecarbonyl derivative and parent isoindoles were antagonists. The 2-ethoxyisoindolo[2,1-a]indoles showed reduced binding affinities compared to their methoxy analogs, while the 5-chloro derivative showed a considerable reduction in binding affinity and potency compared to acetyl 2-methoxyisoindolo[2,1-a]indole compound The 10-methoxy-5,6-dihydroindolo[2,1-a]isoquinolines had higher binding affinities than the corresponding parent indoloisoquinolines in the human receptor subtypes, and the parent compds. were antagonists whereas the 10-methoxy derivs. were agonists in the functional assay. The N-cyclobutanecarbonyl derivs. of both the parent and 10-methoxyl series had similar binding affinities and were both antagonists with similar potencies. The 11-methoxy-6,7-5H-benzo[c]azepino[2,1-a]indoles had higher binding affinities than the corresponding parent compds. at the MT2 receptor but similar affinities at the mt1 site; all of the compds. were antagonists in the functional assay. Changing 11-methoxy for 11-ethoxy decreased the binding affinity slightly, and this was more evident at the MT2 receptor. All of the derivs. investigated had either the same or a greater affinity for the human MT2 receptor compared to the mt1 receptor (range 1:1-1:132). This suggests that the mt1 and MT2 receptor pockets differ in their ability to accommodate alkyl groups in the indole nitrogen

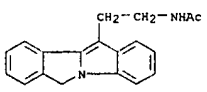
L5 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
region of the melatonin mol. Two compds. were tested in functional assays on recombinant mt1 and MT2 melatonin receptors. N-butanoyl 2-(9-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethanamine was a potent agonist with some selectivity (44-fold) for the MT2 receptor, while N-butanoyl 2-(5,6,7-trihydro-11-methoxybenzo[c]cyclohept[2,1-a]indol-13-yl)ethanamine was an MT2-preferring antagonist. Increasing the carbon chain length between N-1 of indole and the 2-Ph group from n = 1 through n = 3 leads to a fairly regular decrease in the binding affinity, but, remarkably, when n = 3, it converts the methoxy compds. from melatonin agonists to antagonists. The Xenopus melatonin receptor thus cannot accommodate an N-n-alkyl chain attached to a 2-Ph substituent with n > 2 in the required orientation to induce or stabilize the active receptor conformation.

IT 244160-10-9P 263865-08-3P 263865-09-4P
263865-10-7P 263865-11-8P 263865-12-9P
263865-13-0P 263865-14-1P 263865-15-2P
263865-16-3P 263865-17-4P 263865-18-5P
263865-19-6P 263865-20-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and structure of melatonin agonists and antagonists derived from isoindoloindoles, indoloisoquinolines, and benzoazepinoindoles)

RN 244160-10-9 CAPLUS
CN Butanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

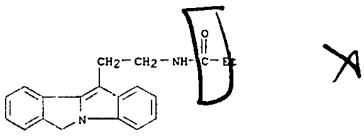


RN 263865-08-3 CAPLUS
CN Acetamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

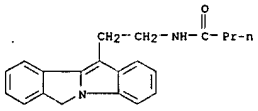


RN 263865-09-4 CAPLUS
CN Propanamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

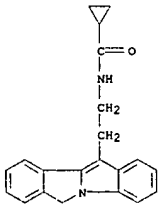
L5 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 263865-10-7 CAPLUS
CN Butanamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

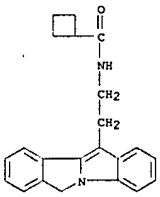


RN 263865-11-8 CAPLUS
CN Cyclopropanecarboxamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

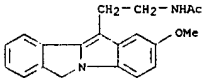


RN 263865-12-9 CAPLUS
CN Cyclobutanecarboxamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI)
(CA INDEX NAME)

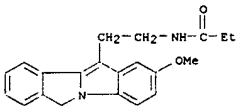
L5 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 263865-13-0 CAPLUS
CN Acetamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

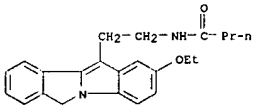


RN 263865-14-1 CAPLUS
CN Propanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

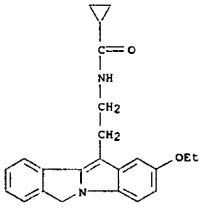


RN 263865-15-2 CAPLUS
CN Cyclopropanecarboxamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

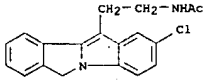
L5 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 263865-19-6 CAPLUS
CN Cyclopropanecarboxamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

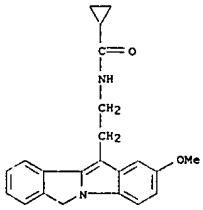


RN 263865-20-9 CAPLUS
CN Acetamide, N-[2-(2-chloro-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

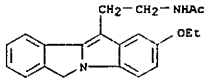


REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

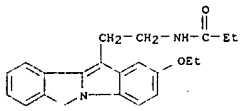
L5 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 263865-16-3 CAPLUS
CN Acetamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



RN 263865-17-4 CAPLUS
CN Propanamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



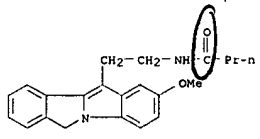
RN 263865-18-5 CAPLUS
CN Butanamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

L5 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:442966 CAPLUS
DOCUMENT NUMBER: 131:240681
TITLE: Design of subtype selective melatonin receptor agonists and antagonists
AUTHOR(S): Sugden, David; Yeh, Li-Kuan; Teh, Muy-Teck
CORPORATE SOURCE: Physiology Division, GKT School of Biomedical Science,
King's College London, London, W8 7AH, UK
SOURCE: Reproduction, Nutrition, Development (1999), 39(3), 335-344
CODEN: RNDEE5; ISSN: 0926-5287
PUBLISHER: Editions Scientifiques et Medicales Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Studies of the physiol. actions of melatonin have been hindered by the lack of specific, potent and subtype selective agonists and antagonists. We describe the utility of a melanophore cell line from Xenopus laevis for exploring structure-activity relationships among novel melatonin analogs and report a novel MT2-selective agonist (IIK7) and MT2-selective receptor antagonist (K185). IIK7 is a potent melatonin receptor agonist in the melanophore model, and in NIH3T3 cells expressing human mt1 and MT2 receptor subtypes. In radioligand binding expts. IIK7 is 90-fold selective for the MT2 subtype. K185 is devoid of agonist activity, but acts as a competitive melatonin antagonist in melanophores. A low concentration (10-9M) antagonizes melatonin inhibition of forskolin stimulation of cAMP in NIH3T3 cells expressing human MT2 receptors, but has no effect in cells expressing mt1 receptors. In binding assays, K185 is 140-fold selective for the MT2 subtype.

IT 244160-10-9
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(melatonin analogs structure-activity relationship in frog melanophore and human melatonin receptors)

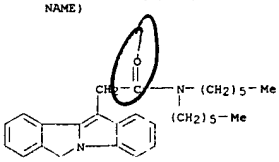
RN 244160-10-9 CAPLUS
CN Butanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



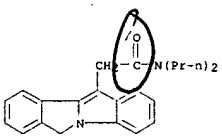
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L5 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:662000 CAPLUS
DOCUMENT NUMBER: 119:262000
TITLE: Chemistry, binding affinities, and behavioral properties of a new class of "antineophobic" mitochondrial DBI receptor complex (mDRC) ligands
AUTHOR(S): Kozikowski, A. P.; Ma, D.; Brewer, James; Sun, S.; Costa, E.; Romeo, E.; Guidotti, A.
CORPORATE SOURCE: Mayo Found. Med. Educ. Res., Jacksonville, FL, 32224, USA
SOURCE: Journal of Medicinal Chemistry (1993), 36(20), 2908-20
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The mitochondrial DBI (diazepam-binding inhibitor) receptor complex (mDRC; previously called the peripheral benzodiazepine receptors) is linked to the production of neurosteroids such as pregnenolone sulfate, dehydroepiandrosterone sulfate, and others. In order to gain further information as to the function of the mDRC in the brain, the authors have constructed and tested, both in vitro and in vivo, a novel series of ligands, 2-arylindole-3-acetamides. The SAR studies detailed herein delineate some of the structural features required for high affinity binding to the mDRCs. In most cases the new ligands were prepared by use of the Fischer indole synthesis. Variations in the length and number of the alkyl groups on the amide nitrogen were probed together with the effects of halogen substituents on one or both of the aryl rings. Some ligands were also synthesized for study which represent conformationally constrained versions of the parent structure. Broad screening studies revealed these indoleacetamides to be highly selective for the mDRC, since they failed to bind with any significant affinity to other receptor systems. Some of the ligands were found to exhibit Ki values in the low nanomolar range for the mDRC as measured by the displacement of [3H]4'-chlorodiazepam. A subset of these ligands was also shown to stimulate pregnenolone formation from the mitochondria of C6-2B glioma cells with an EC50 of about 3 nM. In animal expts. ligands selected for further study were found to exhibit antineophobic effects, in spite of the fact that they exhibit no direct action on GABAA receptors. Consequently, it is postulated that these ligands owe their action to an indirect modulation of GABAA receptor function, presumably by stimulation of neurosteroid production and release from glial cells, followed by neurosteroid modulation of GABA's action on the chloride ion channel conductance of GABAA receptors.
IT 147375-21-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and mitochondrial diazepam-binding receptor complex affinity of, glial neurosteroid release and GABAA receptor function modulation and antineophobic activity in relation to)
RN 147375-21-1 CAPLUS

L5 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 6H-Isoindolo[2,1-a]indole-11-acetamide, N,N-dihexyl- (9CI) (CA INDEX NAME)



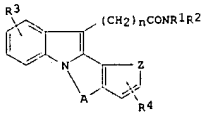
IT 135966-96-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and mitochondrial diazepam-binding receptor complex affinity of, glial neurosteroid release and GABAA receptor function modulation in relation to)
RN 135966-96-0 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-acetamide, N,N-dipropyl- (9CI) (CA INDEX NAME)



L5 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:233880 CAPLUS
DOCUMENT NUMBER: 118:233880
TITLE: Preparation of indolecarboxamides and methods of treating neurological and psychiatric disorders
INVENTOR(S): Costa, Erminio; Guidotti, Alessandro; Kozikowski, Alan; Ma, Dawei
PATENT ASSIGNEE(S): Fidia - Georgetown Institute for the Neurosciences, USA
SOURCE: PCT Int. Appl., 55 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9300334	A1	19930107	WO 1992-US5246	19920626
W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
US 5206382	A	19930427	US 1991-722196	19910627
AU 9222939	A1	19930125	AU 1992-22939	19920626
EP 546164	A1	19930616	EP 1992-914902	19920626
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE				
JP 06501030	T2	19940127	JP 1993-501593	19920626
PRIORITY APPLN. INFO.:			US 1991-722196 A	19910627
			WO 1992-US5246 A	19920626

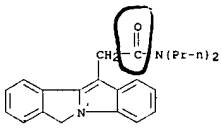
OTHER SOURCE(S): MARPAT 118:233880
GI



I

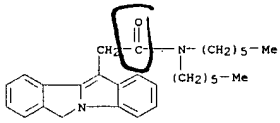
AB Title compds. I [R1, R2 = H, C3-12 alkyl, (alkyl)aryl; R1R2 = 4-6-membered (un)saturated ring; R3, R4 = H, C1-12 alkyl, O2N, H2N, N3, cyano, halo, RO2C, RO, RS (wherein R = H, alkyl); A = C1-3 alkylene to form a ring or null; Z = O, NH, S, CH:CH; n = 1-3] or their salts are prepared PhNHNH2, PhCOCH2CH2CO2H and H2SO4 in EtOH were refluxed for 24 h, cooled and extracted with Et2O to give Et 2-phenyl-3-indoleacetate which in 3N NaOH was refluxed for 3 h, acidified with HCl and treated with Me(CH2)5NH2, PhOP(O)(Cl)NHPh, and Et3N to give I (A = null, Z = CH:CH, R1 = R3 = R4 = H, R2 = hexyl, n = 1). I showed anxiolytic action in rodents at 0.1-0.5 mg/kg.

L5 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
IT 135966-96-0P 147375-21-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as drug for treatment of neurol. disorders and as antipsychotics)
RN 135966-96-0 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-acetamide, N,N-dipropyl- (9CI) (CA INDEX NAME)



– same as #11

RN 147375-21-1 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-acetamide, N,N-dihexyl- (9CI) (CA INDEX NAME)



L5 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:535868 CAPLUS
DOCUMENT NUMBER: 115:135868
TITLE: Palladium catalyzed synthesis of annelated indoles
AUTHOR(S): Kozikowski, Alan P.; Ma, Dawei
CORPORATE SOURCE: Mayo Clin., Jacksonville, FL, 32224, USA
SOURCE: Tetrahedron Letters (1991), 32(28), 3317-20
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 115:135868
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

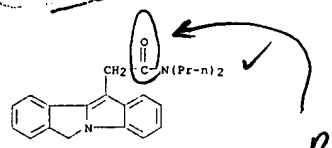
AB The synthesis of polycyclic indoles, e.g., I (X = O, CH2), II, III, is shown to be accomplished readily by the palladium catalyzed intramol. cyclization of bromoarylindoles, e.g., IV, V, VI.

IT 135966-96-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 135966-96-0 CAPLUS

CN 6H-Isoindolo[2,1-a]indole-11-acetamide, N,N-dipropyl- (9CI) (CA INDEX NAME)

same as #10



R_{11} R_{12} #

are acyl